ON SOME APPLICATION OF THE MATHEMATICAL TECHNICS TO VIROLOGY

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ABSTRACT. In this paper we present some connections between mathematics and virology. Moreover, we give the examples of some types viruses, symmetrons with full and effective description of they structure.

1.Introduction.In virology are known (see,[7] pp.171-200) different groups of viruses. One of such groups has been found by Stoltz [9],[10] and by Wrigley [11], [12] and is called as symmetrons. Virus particles are invariably enclosed by shells of protein subunits and these are packed geometrically according to symmetry rules. More of known examples are close packed with each subunit surrounded by six neighbours, except the twelve vertices which have five neighbours. In the paper [2], Goldberg indicated that total number of nearly identical subunits which may be regularly packed on the closed icosahedral surface is given by the following formula:

(G)
$$N = 10T + 2 = 10(a^2 + ab + b^2) + 2$$

where a, b are given non-negative integers and $T = a^2 + ab + b^2$ is the triangulation number for the corresponding symmetron.

Stoltz ([9],[10]) and Wrigley ([11],[12]) discovered that the symmetrons have the construction of linear, triangular and pentagonal and are called:

$$(S-W)_1$$
 disymmetrons, $d_u = u - 1, u = 1, 2, 3, ...$

(S-W)
$$_2$$
 trisymmetrons, $t_v = \frac{(v-1)v}{2}$, $v = 1, 2, 3, ...$

(S-W)₃ pentasymmetrons,
$$p_w = 5\frac{(w-1)w}{2} + 1 = 5t_w + 1, w = 1, 2, 3, \dots$$

Moreover, it is known [11],that an icosahedron has: 30 axes of twofold symmetry, 20 of threefold symmetry and 12 of fivefold symmetry. Hence, the subunits on the surface of an icosahedral virus may be divided into 30, 20 or 12 corresponding previously listed groups symmetry.

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Let the 30 disymmetrons contain d_u subunits, the 20 trisymmetrons contain t_v subunits and the 12 pentasymmetrons contain p_w subunits, then we have

(S-W)
$$N = 10T + 2 = 30d_u + 20t_v + 12p_w$$

where

(1.1)
$$d_u = u - 1$$
, $t_v = \frac{(v - 1)v}{2}$, $p_w = \frac{5w(w - 1)}{2} + 1 = 5t_w + 1$

and u, v, w are positive integers.

For each value of N given by the equation (G) the number f(N) of the solutions of the equation (S-W) is the number

theoretically possible ways of making a virus with N subunits, but with different combinations of symmetrons.

Putting

(1.2)
$$x = 2v - 1$$
, $y = 2w - 1$, $z = u - 1$

and using **(1.1)** in the paper [5] the equation **(S-W)** has been transformed to the following form:

(L)
$$x^2 + 3y^2 + 12z = 4T$$
.

Moreover, in this paper has been proved that total number $f\left(N\right)$ of solutions of the Diophantine equation **(L)** is equal to

(L₁)
$$f(N) = \frac{\pi\sqrt{3}}{180}N + k_1\sqrt{N}$$
,

where k_1 is bounded and is independent of N.

In the same paper in the part entitled "Virological implications" by N.G.Wrigley has been remarked that the only other viruses whose structure is known at present to 1974 are much smaller, N<300, so T<30, thus the virological relevance of this mathematical study is therefore ekstremely speculative.

In this connection has been posed to the solution (see,[5],p.54) of the following problem, which is important for applications in virology:

2. Problem

Find all odd positive integers x, y and all non-negative integers z satisfying the equation (L) for given non-negative integers values of a and b.

In our paper [3] has been given an effective method for the solution of this Problem.Namely,we determine in explicit form positive integers R,S of different parity such that (R,S)=1 and obtain one of such solutions x,y defined by formula,but all other eventuelle solutions of the equation (L) could be determined by specific computation. The symbol (R,S)=1 denote that the positive integers R,S of different parity have the greatest common divisor equal to 1. For such

computation we can applied of the following inequalities: $x < 4 \max\{R,S\}$, $y < 3 \max\{R,S\}$.

In our paper [4] has been given complete solution of the **Problem**.Namely,we obtain the explicit formulas giving all solutions in odd, positive integers x,y of the equation (**L**) for each fixed non-negative integer $z \in [0, \frac{1}{3}T)$, where $T = a^2 + ab + b^2$ is given triangulation number.

First, we note that the Diophantine equation **(L)** we can present in the following form:

(2.1)
$$x^2 + 3y^2 = 4(T - 3z)$$
,

where $T = a^2 + ab + b^2$, and a, b are given non-negative integers.

Since $x^2 + 3y^2 > 0$ and $z \ge 0$, then by (2.1) it follows that

(2.2)
$$0 \leqslant z < \frac{1}{3}T$$
.

For given non-negative a, b the triangulation number $T = a^2 + ab + b^2$ is fixed integer. Therefore, there exist finite number of integers z satisfying the inequality (2.2).

Let $z=z_0\in[0,\frac{1}{3}T)$ and $T_0=T-3z_0$ then the equation (2.1) reduces to the following form:

$$(2.3) x^2 + 3y^2 = 4T_0.$$

Since T_0 is positive integer then by application some results of number theory (see; [1],p.91 and [8], p.221;p.349) we can presented it in the form:

$$(2.4) T_0 = R^2 + 3S^2$$

where R, S are different parity positive integers unique determined such that have greatest common divisor equal to one.

From (2.3) and (2.4) follows that the equation (2.1) has the following form:

(L-G)
$$x^2 + 3y^2 = 4(R^2 + 3S^2)$$
,

where R, S are different parity positive integers such that (R, S) = 1.

In our paper [4] has been proved of the following Theorem:

Theorem. All solutions in odd, positive integers x, y of the equation:

(L-G)
$$x^2 + 3y^2 = 4(R^2 + 3S^2)$$
,

where R,S are given positive integers, different parity and relatively prime are given by the formulas:

(L-G)*
$$x_1 = |R - 3S|, y_1 = R + S \text{ and } x_2 = R + 3S, y_2 = |R - S|.$$

This **Theorem** give full solution of the **Problem** posed in the paper [4]. **Remarks**

Remark1. If the equation **(L)** has a solution in odd positive integers x, y then the number T-3z on the right hand of the equation (2.1) must be odd non-negative integer.

Therefore, if T is an odd positive integer, then it suffices to consider only even, non-negative integers $z \in [0, \frac{1}{3}T)$.

Similarly, if T is an even positive integer, then it suffices to consider only odd non-negative integers $z \in [0, \frac{1}{3}T)$.

Remark 2. J.E.Johnson and W.Chiu in the paper [5] give an example of an virus with icosahedral symmetry having the triangulation number T > 30.

This virus is called "PARAMAECIUM BURSARIA CHLORELLA VIRUS" and has the triangulation number $T=169.\mathrm{In}$ the paper [4] has been given the full description of the structure for this virus.

3. Some examples of the symmetrons with the mathematical description of they structures.

In this paper we give further application of the mathematical technic by using of the **Theorem** to the full desription of the following symmetrons:

I.Reovirus : T=13,**II. Herpesvirus:** T=16, **III. Adenovirus:** T=25.

I.Reovirus.

The triangulation number T=13 is odd positive integer, hence by **Remark 1** it follows that it suffices to consider the even number z=0,2,4.

For z=0,we have $T_0=T=13=1^2+3\cdot 2^2$.Hence R=1,S=2 and consequently by the **Theorem** it follows that equation **(L-G)** has the following solutions in odd positive integers:

(3.1)
$$x_1 = |R - 3S| = 5, y_1 = R + S = 3$$
 and $x_2 = R + 3S = 7, y_2 = |R - S| = 1$

For z = 2 we have $T_0 = T - 3z = 13 - 6 = 7 = 2^2 + 3 \cdot 1^2$, hence R = 2, S = 1. Therefore we get

(3.2)
$$x_1 = |R - 3S| = 1, y_1 = R + S = 3$$
 and $x_2 = R + 3S = 5, y_2 = |R - S| = 1$.

For z=4 we have $T_0=T-3z=13-3\cdot 4=13-12=1$. This case is impossible, because the numer 1we can not presented in the form $1=R^2+3S^2$, with positive integers such that (R,S)=1.

Now, by application of the formulas (1.2) and $(S-W)_1$ - $(S-W)_3$ we can determined the number of the disymmetrons, trisymmetrons and pentasymmetrons in the structure of the viuse I. For the case z=0, we have

(3.3)
$$x_1 = 2\nu - 1 = 5, y_1 = 2\omega - 1 = 3, z = u - 1 = 0.$$

From (3.3) we get that

(3.4)
$$\nu = 3, \omega = 2, u = 1$$

By (3.4) and $(S-W)_1$ - $(S-W)_3$ it follows that

(3.5)
$$d_u = u - 1 = 0, t_\nu = \frac{(\nu - 1)\nu}{2} = 3, p_\omega = 5 \cdot \frac{(\omega - 1)w}{2} + 1 = 6.$$

From (3.5) and the formula (S-W) we get that

$$N = 10T + 2 = 10 \cdot 13 + 2 = 132 = 30d_u + 20t_\nu + 12p_\omega = 30 \cdot 0 + 20 \cdot 3 + 12 \cdot 6 = 60 + 72 = 132.$$

In similar way for the second case of the solutions given in (3.1) we obtain

(3.6)
$$d_{\nu} = 0, t_{\nu} = 6, p_{\omega} = 1.$$

From (3.6) we have
$$N = 30 \cdot 0 + 20 \cdot 6 + 12 \cdot 1 = 120 + 12 = 132$$
.

In the case (3.2) we obtain for $x_1=1,y_1=3$ that $\nu=1,\omega=2,u=3,$ and consequently we have

(3.7)
$$d_u = 2, t_\nu = 0, p_\omega = 6.$$

From (3.7) we get that
$$N = 30 \cdot 2 + 20 \cdot 0 + 12 \cdot 6 = 60 + 72 = 132$$
.

For the second solution of the case (3.2) we have $x_2=5, y_2=1,$ hence $\nu=3, \omega=1, u=3.$ Therefore we obtain

(3.8)
$$d_u = 2, t_\nu = 3, p_\omega = 1.$$

From (3.8) we have that
$$N = 30 \cdot 2 + 20 \cdot 3 + 12 \cdot 1 = 60 + 60 + 12 = 132$$
.

From the mathematical calculations follows that the symmetron called as the **Reovirus** with the triangulation number T=13 has the following structure with respect to the number of the disymmetrons d_u , trisymmetrons t_v and pentasymmetrons p_ω :

d_u	$t_{ u}$	p_{ω}	$z=z_0$
0	3	6	0
0	6	1	0
2	0	6	2
2	3	1	2

By similar calculations we obtain the full ad effective form of the structure for the **Herpesvirus** and **Adenovirus**. The final results we present in the correspondig Tables.

II. Herpesvirus

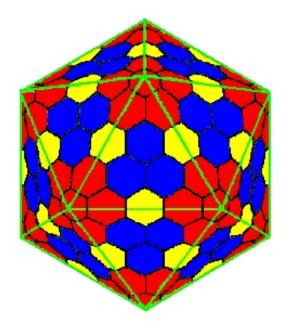
Since T=16 thus we see by the **Remark 1** that z is odd nmuber such that $0\leqslant z<\frac{16}{3}$, hence z=1,3,5.For $z=z_0=5$ we have that $T_0=T-3z=16-3\cdot 5=1.$

This case is impossible , because $1 \neq R^2 + 3S^2$ for positive integers R,S such that (R,S)=1.

Hence, we have

$z = z_0$	$T_0 = T - 3z_0$	$T_0 = R^2 + 3S^2$	R	S	x_1	y_1	x_2	y_2
1	$T_0 = 16 - 3 = 13$	$13 = 1^2 + 3 \cdot 2^2$	1	2	5	3	7	1
3	$T_0 = 16 - 3 \cdot 3 = 7$	$7 = 2^2 + 3 \cdot 1^2$	2	1	1	3	5	1

z_0	d_{ν}	t_{ν}	p_{ω}	$N = 30 \cdot d_u + 20 \cdot t_\nu + 12 \cdot p_\omega$
1	1	3	6	$N = 30 \cdot 1 + 20 \cdot 3 + 12 \cdot 6 = 162$
1	1	6	1	$N = 30 \cdot 1 + 20 \cdot 6 + 12 \cdot 1 = 162$
3	3	0	6	$N = 30 \cdot 3 + 20 \cdot 0 + 12 \cdot 6 = 162$
3	3	3	1	$N = 30 \cdot 3 + 20 \cdot 3 + 12 \cdot 1 = 162$



The graphic presentation of the **Herpesvirus** with the triangulation number T=16 has $d_u=1, t_\nu=3, p_\omega=6$. Pentasymmetrons have the colour red, trisymmetrons have the colour blue and disymmetrons have the colour yellow.

III. Adenovirus

Since this virus has the triangulation number T=25,hence it suffices consider only even numbers $0\leqslant z<\frac{25}{3}$.

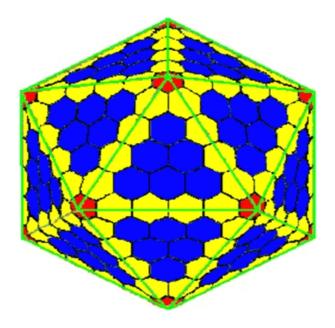
Consequently , we consider the numbers $z=z_0=0,2,4,6,8.$ If $z=z_0=0,$ then we have $T_0=T-3z=25\neq R^2+3S^2.$

Similarly, if $z=z_0=8$ then we have $T_0=1\neq R^2+3S^2$. We see that this two cases are imposible. Hence, we have

$z = z_0$	$T_0 = T - 3z_0$	$T_0 = R^2 + 3S^2$	R	S	x_1	y_1	x_2	y_2
2	$T_0 = 19$	$19 = 4^2 + 3 \cdot 1^2$	4	1	1	5	7	3
4	$T_0 = 13$	$13 = 1^2 + 3 \cdot 2^2$	1	2	5	3	7	1
6	$T_0 = 7$	$7 = 2^2 + 3 \cdot 1^2$	2	1	1	3	5	1

$z=z_0$	d_u	t_v	p_{ω}	$N = 30 \cdot d_u + 20 \cdot t_\nu + 12 \cdot p_\omega$
2	2	0	16	$N = 30 \cdot 2 + 20 \cdot 0 + 12 \cdot 16 = 252$
2	2	6	6	$N = 30 \cdot 2 + 20 \cdot 6 + 12 \cdot 6 = 252$
4	4	3	6	$N = 30 \cdot 4 + 20 \cdot 3 + 12 \cdot 6 = 252$
4	4	6	1	$N = 30 \cdot 4 + 20 \cdot 6 + 12 \cdot 1 = 252$
6	6	0	6	$N = 30 \cdot 6 + 20 \cdot 0 + 12 \cdot 6 = 252$
6	6	3	1	$N = 30 \cdot 6 + 20 \cdot 3 + 12 \cdot 1 = 252$

The graphic presentation of the **Adenovirus** with triangulation number T=25.Pentasymmetrons $p_{\omega}=1$ have the colour red,trisymmetrons $t_{\nu}=6$ have the colour blue and disymmetrons $d_{u}=4$ have the colour yellow



REFERENCES

- [1] L.E.Dickson, Introduction to the Theory of Numbers, Dover Publ.New York, 1957.
- [2] M.Goldberg, A class of multi-symmetric polyhedra, Tohoku Math.J. 43 (1937), 104 108
- [3] A.Grytczuk, Ljunggren's Diophantine problem connected with viruse structure, Annales Math.et Informaticae, 33 (2006), 69-75.
- [4] A.Grytczuk and K.Grytczuk, Application of Ljunggren's Diophantine equation to the description of the viruses structure, International J.Appl. Math. and Applications, Vol. 2 No. 1 (2019), 35-42
- [5] W.Ljunggren, *Diophantine analysis applied to virus structure*, Math.Scand.34 (1974),51-57 (presented by N.G.Wrigley and V.Brun)
- [6] J.E.Johnson and W.Chiu, Structures of virus and virus-like particles, Current Opinion in Structural Biology, 10 (2000), 229-235.
- [7] H.G.Schlegel, Mikrobiologia ogólna, PWN, Warszawa, 2005 (Polish Edition-Allgemeine Mikrobiologie, Georg Thieme Verlag, Stuttgart, 1992)
- [8] W.Sierpiński, Elementary Theory of Numbers, PWN, Warszawa, 1987 (Editor: A.Schinzel)
- [9] D.B.Stoltz, The structure of icosahedral cytoplasmic Deoxyriboviruses, J. Ultrastruct. Res. 37 (1971), 219-239
- [10] D.B.Stoltz, The structure of icosahedral cytoplasmic Deoxyriboviruses, II: An alternative model, J.Ultrastruct.Res.43(1973),58-74.
- [11] N.G.Wrigley, An electron microscope study of the structure of Sericesthis iriddescent virus, J.gen.Virol. (1969),123-134.
- [12] N.G.Wrigley, An electron microscope study of the structure of Tipula iridescent virus, J.gen. Virol. 6(1969), 169-173.

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